Physics in a Nano-Scale

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Abstract

Since much attention is being drawn to nano-optoelectronic devices, with promising technological and medical applications (molecular photosensitization, colour-dyes, new generation of solar cell applications, Li-ion batteries), the understanding of the electrical and optical properties of hydrogen-passivated silicon nanocrystals (Si-NC) becomes an important aspect to focus upon, due to the fact that these systems possess different properties from those of the bulk materials.

Nanostructures, smaller than macroscopic objects (present-day electronic devices), but larger than molecules, which description belongs to a complex domain of quantum mechanics, where amazing properties emerge.

Quantum effects become dominant when the nanometre size range is reached, thus accounting for changes in the physical properties of nanostructures, as is the case for the increase in surface area to volume ratio altering mechanical and thermal properties of materials. Here, the geometry of the material can dictate drastic effects on quantized states.

In the bulk mode, silicon has an indirect, low energy gap of 1.1 eV, in the infra-red region [1]. The indirect radiative interband transitions suppresses the electron-hole radiative recombination, hence making silicon a poor light emitter.

As the size of the Si decreases, reducing into a finite sized material (nano-scale), the energy difference between energy states and the energy band-gap tends to widen, driving the lowest occupied and the highest occupied energy states further apart. This will give the small nanocrystals a direct gap-like behaviour [3] with discrete energy spectra, confining the charge carriers within the dimensions of the nano-structure. The strong spatial localization of electrons and holes in Si-NCs can enhance radiative recombination rates and give rise to luminescence [2].

The band-gaps for the hydrogen-terminated nanosystems will be strongly dependant on the size of the system, due to the quantum confinement effects. The greater the difference between the lowest occupied and the highest occupied energy states, more energy is needed to excite the nanocrystal, and therefore, more energy is released when the system relaxes to its fundamental state. This will result in a colour shift from red to blue of the emitted light [4].

Another form of controlling the electronic and optical properties of Si-NC is by altering its chemical composition, for example by introducing impurities in the material [5]. Doped nanocrystals may emit light different than those emitted by pure NC, indicating that the impurity level affects the absorption and photoluminescence spectra.

Phosphorous and Boron are the most studied dopants in Si (as they are easier to incorporate) and thus their binding energies, as shallow impurities, are well established for the bulk Si semiconductor. In bulk Si, these impurities introduce defect energy states close to the conduction and valence band, respectively, enabling thermal excitation of the charge carriers, thus enhancing the conductivity of the material and altering the respective transport properties [7].

Reducing the dimensionality of the system, the defect's electric levels start to deepen into the mid gap, being this an evidence of how the size of the nanocrystal affects the localization of the defect states [1]. The combined effects of both quantum confinement and weak screening (the dielectric screening is different at decreasing length scales) thus modify well established shallow impurities of the bulk, into deep levels in the nanocrystals [1].

Moreover, doping in nanostructures is more problematic than in bulk materials. One of the main difficulties is the control over impurity concentration and precise positioning, because of the out-of-phase relation of impurity concentrations between nano and bulk-sized materials - a small amount of dopant atoms can correspond to higher impurity concentrations in a nanomaterial [7]. Increasing dopant concentration results in distinct changes in the photoluminescence properties due to the influence on the mobility of the charge carriers [8].

Another difficulty that arises in doping nanomaterials is the deactivation of the functionalization properties (self-purification) of the impurity atoms. These foreign atoms can be expelled or segregated to the surface of the host material due to energetic and kinetic processes, that result from the effects of the confined dimensions [7].

The possibility for atomic manipulation is one of the main advantages of Si-NC, which allows the control over the conductive and optical properties of the material. Since the new generation of optoelectronic devices is being drawn towards the nanometre, it becomes crucial to understand the quantum confinement effects of pure NC. It is also imperative to search for suitable impurities which can contribute with electronic, optical or magnetic performance at the nanoscale, because the presence of single donor and acceptor states can lower the energy gap of the pure Si-NC [6, 1], whereas deep defects may degrade device performance.

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